

CONVEX TREE REALIZATIONS OF PARTITIONS

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Abstract—Given a collection P of partitions of a label set L a problem arising in biological and linguistic classification is deciding whether there is a “tree-structure” on L which is “compatible” with P . While this problem is, in general, NP -complete we show that it has a polynomial time solution if the number of sets in each partition is at most three.

1. INTRODUCTION

A problem arising in certain branches of classification such as taxonomy [1] is to determine whether a collection of partitions of some label set has a tree-like representation in a sense which we will define shortly. In order to do this, and to place this question in a context which relates it to a simpler problem in which the partitions are already endowed with some tree-like structure we must first make a number of definitions.

- (1) Given a tree $T = (V(T), E(T))$ and a subset A of $V(T)$ let $\langle A \rangle_T$ denote the minimal connected subset of $V(T)$ which contains A .
- (2) A *semilabelled tree* on L is a pair $\tau = (T, f)$ where T is a tree, $f : L \rightarrow V(T)$ is a map, and if $v \notin f(L)$ then $\deg(v) > 2$. Two such pairs $\tau = (T, f)$ and $\tau' = (T', f')$ are considered identical if there is a tree isomorphism $H : V(T) \rightarrow V(T')$ with $f' = H \circ f$.
- (3) A partition X of L into disjoint subsets a, b, \dots , is *convex* on a semilabelled tree $\tau = (T, f)$ if for all $a, b \in X, a \neq b, \langle f(a) \rangle_T \cap \langle f(b) \rangle_T = \emptyset$.
- (4) A collection P of partitions of L is *compatible* if there exists a semilabelled tree τ on which each partition is convex (we say τ is compatible with P).
- (5) Given two trees T, T' a function $h : V(T) \rightarrow V(T')$ is a *contraction* if T' is obtained (up to isomorphism) by collapsing edges of T , and h is the induced vertex identification map.
- (6) For semilabelled trees $\tau = (T, f), \tau' = (T', f')$ we say τ is a *refinement* of τ' if there is a contraction $h : V(T) \rightarrow V(T')$ satisfying $f' = h \circ f$.
- (7) A collection S of semilabelled trees on L are *compatible* if there exists a semilabelled tree τ which is a refinement of each semilabelled tree in S (we say τ is compatible with S).
- (8) A semilabelled tree $\tau = (T, f)$ on L defines a partition $\pi(\tau)$ of L by setting $\pi(\tau) = \{f^{-1}(\{v\}) : v \in V(T), f^{-1}(\{v\}) \neq \emptyset\}$.
- (9) Given a semilabelled tree $\tau = (T, f)$ deleting any edge $e \in E(T)$ partitions $V(T)$ into two connected subsets; applying f^{-1} to these sets partitions L into at most two sets. Let β_τ be the set of bipartitions of L which can be generated in this way from τ . For a set S of semilabelled trees on L let $B(S) = \cup_{\tau \in S} \beta_\tau$.
- (10) Following Buneman [2] a set $B = \{\sigma_1, \dots, \sigma_k\}$ of bipartitions of L defines a connected graph $G[B] = (V, E)$, and a labelling function $f : L \rightarrow V$ as follows: V consists of all sets $v = \{S_1, \dots, S_k\}$ where $S_i \in \sigma_i$ and $S_i \cap S_j \neq \emptyset$ for all i, j . Two such sets v, v' are the ends

of an edge in E precisely if $|v \cap v'| = k - 1$. For $v \in V, v = \{S_1, \dots, S_k\}$, let $I_v = \bigcap_i S_i$. Then it can be checked that $\{I_v : v \in V, I_v \neq \emptyset\}$ partitions L , and thus the function

$$f : L \rightarrow V, \\ f(x) = \{S_1(x), \dots, S_k(x)\}, \text{ with } x \in S_i(x) \in \sigma_i,$$

is well defined and its range contains all $v \in V$ of degree at most two.

In taxonomy, a partition of L is called an "unordered qualitative character", while a semilabelled tree is called an "undirected cladistic character". In taxonomic and other applications an important class of semilabelled trees (T, f) are *phylogenetic trees*, for which f is a bijection from L onto the degree one vertices of T . In case all the remaining vertices of T have degree 3, (T, f) is called a *binary* (or *nondegenerate*) *phylogenetic tree*.

2. PRELIMINARIES

The following result summarizes the fundamental relationships between the definitions introduced above. Most of (2) is due to Buneman [2]; see also Barthélemy [3]. Result (3a) follows from the first part of (1) and the observation that a bipartition σ is convex on τ precisely if $\sigma \in \beta_\tau$, while (3b) follows from (2b). Result (5) was stated by Buneman [4] and Meacham [1]. The remaining results are largely part of the folklore (see, for example [5]).

THEOREM 1.

- (1) τ is a refinement of τ' precisely if $\beta_\tau \supseteq \beta_{\tau'}$. Furthermore, $\beta_\tau = \beta_{\tau'}$ implies $\tau = \tau'$; thus semilabelled trees are partially ordered by refinement.
- (2a) Two bipartitions $\{A_1, A_2\}, \{B_1, B_2\}$ are compatible precisely if $\emptyset \in \{A_i \cap B_j : i, j \in \{1, 2\}\}$.
- (2b) $G[B]$ is a tree precisely if B is pairwise compatible. In this case $\tau(B) := (G[B], f)$ is a semilabelled tree which is compatible with B ; $\beta_{\tau(B)} = B$; any other semilabelled tree compatible with B is a refinement of $\tau(B)$, and (assuming B has no repeated bipartitions) $G[B]$ has $|B| + 1 < 2|L| - 2$ vertices.
- (3a) A collection S of semilabelled trees is compatible (with τ) if and only if the induced bipartitions $B(S)$ are compatible (with τ).
- (3b) A collection B of bipartitions is compatible (with τ) if and only if B is pairwise compatible (with τ).
- (4) A collection P of partitions is compatible (with τ) if and only if there exists a collection S_P of semilabelled trees which is compatible (with τ) and such that $P = \{\pi(\tau) : \tau \in S_P\}$. Furthermore in case P is compatible we may insist, for each $(T, f) \in S_P$, that f is surjective.
- (5) A collection P of partitions is compatible if and only if the intersection graph of the set system $\bigcup_{X \in P} X$ can be transformed into a chordal graph by introducing additional edges, but subject to the restriction that vertices a, a' remain non-adjacent if for some $X \in P, a, a' \in X$.
- (6) If a collection of partitions or of semilabelled trees are compatible then the collection is compatible with a binary phylogenetic tree (as defined in the introduction).

Combining 3(a) and 3(b) gives the following result, due to Estabrook, Johnson and McMorris [6].

COROLLARY 1. "The Pairwise Compatibility Theorem" A collection S of semilabelled trees is compatible if and only if it is pairwise compatible. Indeed, by Theorem 1, there is a unique semilabelled tree which is both compatible with S and minimal with respect to refinement, namely $(G[B(S)], f)$.

Applying Theorem 1(5) it is easily shown that two partitions are compatible precisely if the bipartite intersection graph of the two partitions is acyclic, a result proved explicitly by Estabrook and McMorris [7].

3. AN EXTENSION

By the above corollary, the compatibility of a set of semilabelled trees can be established in polynomial time. In particular, as is well known, deciding whether a collection B of bipartitions of L is compatible, and constructing a compatible tree, can be carried out in polynomial time (see [8] or [9] for an $O(|L| \times |B|)$ algorithm).

Polynomial time also applies if a bound is placed on the number of partitions. However, deciding whether an arbitrary set of partitions is compatible is NP -complete, even if each set in each partition has cardinality at most two [10]. A natural question then is whether the compatibility of sets of partitions, each having a bounded number of sets, can be decided in polynomial time. Corollary 2 (below) answers this affirmatively in case each partition has at most three sets. It is not known whether the same applies if each partition has at most k sets (for fixed k), even when $k = 4$. Recall that a star-shaped tree is a tree having all but one of its vertices of degree 1.

THEOREM 2. *For a collection P of partitions of L constructing a compatible collection S_P of star-shaped semilabelled trees such that $P = \{\pi(\tau) : \tau \in S_P\}$, or deciding that no such collection exists, can be achieved in $O(|L| \times p^2)$ time, where $p = \bigcup_{X \in P} |X|$.*

PROOF. Regard the sets occurring in at least one partition in P as the vertices of a graph G , in which two sets A, B are joined by an edge of G precisely if $\{A, A'\}$ and $\{B, B'\}$ are incompatible partitions (here $'$ denotes complement). Note that each partition is an independent set of vertices of G (that is, no two vertices are adjacent). Also, deciding whether an edge exists between two vertices takes $O(|L|)$ time, and there are $O(p^2)$ pairs of vertices, so G can be constructed in $O(|L| \times p^2)$ time. For $X \in P$ there is a natural bijection λ_X from $X^* := \{V : V \subseteq X, |V| \geq |X| - 1\}$ to $\{\beta_\tau : \tau \text{ is star-shaped, } \pi(\tau) = X\}$, namely

$$\lambda_X(\{A_1, \dots, A_s\}) := \{\{A_1, A_1'\}, \dots, \{A_s, A_s'\}\}, s = |X| \text{ or } |X| - 1.$$

By the definition of G , if $V_X \in X^*$ for all $X \in P$, then $\cup \lambda_X(V_X)$ is pairwise compatible precisely if $\cup V_X$ is an independent set of vertices in G . Thus by Theorem 1(3) the collection S_P in the statement of the theorem exists precisely if G has an independent set of vertices containing at least $|X| - 1$ vertices from each $X \in P$. We now describe a simple procedure which finds such an independent set if it exists. Essentially we describe a way of building up a set I , which is always an independent set, by testing the effect of adding one more new vertex. Set $I = \emptyset$ and while there exists $X \in P$, with $|I \cap X| < |X| - 1$ select $x \in X - I$, and let $A := \{x\}, B := \emptyset$. Apply the following rule:

\mathcal{R} : While

- (1) $A \cap B = \emptyset$ and
- (2) there exists $a \in A$ which is adjacent to $y \notin B$,

then replace A and B by $A \cup \bigcup_{y \in Y \in P} (Y - \{y\})$ and $B \cup \{y\}$, respectively.

Eventually, in $O(p)$ steps, either (1) or (2) fails. If (2) fails but not (1), then replace I by $I \cup A$. If (1) fails replace A and B by $\bigcup_{x \in X \in P} X - \{x\}$ and $\{x\}$ respectively, and apply rule \mathcal{R} again, and in this case if (2) fails but not (1) then again replace I by $I \cup A$, while if (1) fails then no independent set of the type required can exist (since it would have to simultaneously include and exclude x). Thus, provided this does not occur, $|I|$ is enlarged by at least one element, and, by induction, all the elements of I are non-adjacent. Thus, in $O(p)$ steps, the procedure described gives the required independent set.

Since every semilabelled tree τ with $|\pi(\tau)| \leq 3$ is star shaped, combining Theorem 2 with part (4) of Theorem 1, and applying a reconstruction algorithm, like that described in [9], we obtain the following.

COROLLARY 2. *If P is a collection of partitions of L into at most three disjoint sets then constructing a semilabelled tree which is compatible with P , or deciding that no such tree exists can be achieved in $O(|L| \times |P|^2)$ time.*

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